Math

UIUCDCS-R-78-931

UILU-ENG 78 1723
COO-2383-0048

STABILITY OF VARIABLE-STEP METHODS FOR ORDINARY DIFFERENTIAL EQUATIONS

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Supported in part by the Department of Energy under grant ENERGY/EY-76-S-02-2383.

1. Introduction

In a recent report, Zlatev [4] extends the known class of unconditionally stable variable-step multistep methods (that is, methods which are stable for any stepsize sequence such that the ratio of the largest to smallest steps is bounded) to include methods of the form

$$(1.1) \qquad y_n = \alpha_1[\{h\}]y_{n-1} + \alpha_2[\{h\}]y_{n-2} + \text{derivative terms.}$$

By the notation $\alpha_i[\{h\}]$ we simply indicate that the α_i may depend on the ratio of one or more past steps. Zlatev shows (1.1) to be stable as long as $|\alpha_2| < 1$, a property that will hold for any reasonable strategy for computing α_1 and α_2 from $\{h\}$. (Note that $|\alpha_2| < 1$ for a strongly stable constant-step method.)

The proof of convergence presented in Zlatev's report is particularly interesting for two reasons: (a) it yields a proof of fixed-step convergence that is intuitively more pleasing than the "standard" proof, as found in Henrici [3], being more direct; and (b) it permits an extension to all strongly stable methods, which, while not yielding unconditional stability (shown to be untrue in general by a counter example in [1]), leads to a bound on stepsize ratios which can be computed for any particular formula, and hence simply implemented in practical programs.

This short paper discusses an extension of Zlatev's proof, first at an intuitive level which this writer finds particularly appealing, then at a technical level. Finally, the constructive application of the result to the calculation of stable-step ratios (the bounds b and B) is discussed.

2. Zlatev's Proof Technique

Consider the strongly stable, constant-step method

(2.1) $$y_n = \sum_{i=1}^{k} \alpha_i y_{n-i} + \sum_{i=0}^{k} h\beta_i f(y_{n-i})$$

for the initial value problem

(2.2) $$y' = f(y, t), \qquad y(0) = y_0.$$

The equation for the global error, $e_n = y_n - y(t_n)$, takes the form

(2.3) $$e_n = \sum_{i=1}^{k} \alpha_i e_{n-i} + \sum_{i=0}^{k} h\beta_i g_{n-i} e_{n-i} + d_n ,$$

where $g_j = f_y$ evaluated at a suitable point, and d_n is the local truncation error. The "standard" proof of convergence involves bounding the rate of growth of solutions of this difference equation which is an order h perturbation of a difference equation with a root at one. Zlatev considers, instead, a difference equation for $c_n = e_n - e_{n-1}$. This satisfies the equation

(2.4) $$c_n = e_n - e_{n-1} = \sum_{i=1}^{k-1} \gamma_i c_{n-i} + \sum_{i=0}^{k} h\beta_i g_{n-i} e_{n-i} + d_n$$

If we write $\rho(\xi) = -\xi^k + \sum_{i=1}^{k} \alpha_i \xi^{k-i}$, $\bar{\rho}(\xi) = -\xi^k + \sum_{i=1}^{k-1} \gamma_i \xi^{k-i}$ we find that $\bar{\rho}(\xi) = \xi\, \rho(\xi)/(\xi-1)$, that is, $\bar{\rho}(\xi)$ is a "deflated" form of $\rho(\xi)$ with the unit root replaced by zero. If the method is strongly stable, $\bar{\rho}(\xi)$ has all of its zeros strictly inside the unit circle, hence the growth of solutions of eq. (2.4) can be bounded by a constant times the largest of the added terms $(\sum_{i=0}^{k} h\beta_i g_{n-i} e_{n-i} + d_n)$. If d_n is $O(h^{p+1})$ and e_n is $O(h^p)$, this term is $O(h^{p+1})$, hence c_n is $O(h^{p+1})$. The global

error e_n is simply $e_0 + \sum_{i=1}^{n} (c_i)$, and, since there are order of $1/h$ terms in the sum, e_n is $O(h^{p+1}/h) = O(h^p)$. Of course, this argument is circular, so there are a few technical details to work out. This is the subject of the next section.

3. Variable-step Methods

Consider a method given by eq. (2.1) where h depends on n, and the α_i and β_i may vary with the ratios of stepsizes. Following the notation in [1], the error equation (2.3) may be written in the form

$$\underline{e}_n = (S_n + h_n \tilde{S}_n)\underline{e}_{n-1} + \underline{d}_n \tag{3.1}$$

where $\underline{e}_n$ is the error in the collection of saved information $\underline{y}_n$ (e.g., $\underline{y}_n = [y_n, y_{n-1}, y_{n-2}, \ldots, h_n y_n', h_{n-1} y_{n-1}', \ldots]^T$), $\tilde{S}_n$ contains the dependence of (2.3) on $g = \partial f/\partial y$, and S_n depends only on the coefficients of the method. In [1] it is shown that if $||S_m^n||$ (where $S_m^n = \prod_{j=m+1}^{n} S_j = S_n S_{n-1} \cdots S_{m+1}$) and $||\tilde{S}_n||$ can be bounded independently of $n > m$, then convergence can be proved for consistent methods, so that bounded $||S_m^n||$ and $||S_n||$ is a reasonable <u>stability condition</u>. For the multistep method above,

$$
S_n = \left[\begin{array}{ccccc|ccccc}
\alpha_1 & \alpha_2 & \cdots & & \alpha_k & \beta_1 & \beta_2 & \cdots & & \beta_k \\
1 & 0 & \cdots & & 0 & & & & & \\
0 & 1 & \cdots & & 0 & & & \bigcirc & & \\
\vdots & & \ddots & & \vdots & & & & & \\
0 & 0 & & 1 & 0 & & & & & \\
\hline
 & & & & & 0 & 0 & \cdots & & 0 \\
 & & & & & 1 & 0 & \cdots & & 0 \\
 & & \bigcirc & & & 0 & 1 & \cdots & & 0 \\
 & & & & & \vdots & & \ddots & & \vdots \\
 & & & & & 0 & 0 & & 1 & 0
\end{array}\right]
$$

We now consider the similarity transformation of S_n to $Q\ S_n\ Q^{-1}$ where

$$
Q = \left[\begin{array}{ccccc|ccc}
1 & 0 & \cdots & & 0 & & & \\
-1 & 1 & \cdots & & 0 & & \bigcirc & \\
 & \ddots & \ddots & & & & & \\
\bigcirc & & & -1 & 1 & & & \\
\hline
 & & & & & 1 & & \\
 & & \bigcirc & & & & \ddots & \\
 & & & & & & & 1
\end{array}\right]
$$

This corresponds to a change of variables, from e_n, e_{n-1}, $e_{n-2}, \ldots$ to e_n, $-c_n$, $-c_{n-1}, \ldots$ and is in the spirit of Zlatev's technique. We find that

$$
Q\,S_n\,Q^{-1} = \left[\begin{array}{c|cccc|cccc}
1 & -\gamma_1 & -\gamma_2 & \cdots & -\gamma_{k-1} & \beta_1 & \beta_2 & \cdots & \beta_k \\
0 & \gamma_1 & \gamma_2 & \cdots & \gamma_{k-1} & -\beta_1 & -\beta_2 & \cdots & -\beta_k \\
0 & 1 & 0 & & 0 & & & & \\
 & & \ddots & & & & \bigcirc & & \\
 & & & 1 & 0 & & & & \\
\hline
 & & & & & 0 & 0 & \cdots & 0 \\
 & & & & & 1 & 0 & & 0 \\
 & & \bigcirc & & & 0 & 1 & & 0 \\
 & & & & & & & \ddots & \\
 & & & & & & & 1 & 0
\end{array}\right]
$$

$$
= \left[\begin{array}{c|c|c}
1 & x_n & \\
\cline{1-2}
0 & \hat{S}_n & B_n \\
\hline
\multicolumn{2}{c|}{\bigcirc} & C
\end{array}\right]
$$

Hence, $Q\, S_m^n\, Q^{-1} = \prod_{j=m+1}^{n} (Q\, S_j\, Q^{-1})$

$$= \left[\begin{array}{c|c|c} 1 & y_{n,m} & \\ \cline{1-2} 0 & \hat{S}_m^n & B_{n,m} \\ \hline \multicolumn{2}{c|}{\bigcirc} & C^{n-m} \end{array}\right]$$

where

(3.2) $$y_{n,m} = y_{n-1,m} + x_n\, \hat{S}_m^{n-1} \quad \text{with } y_{mm} = 0 \ .$$

Suppose, for a moment, that $||\hat{S}_n^p|| \leq r$ where $r < 1$. Then eq. (3.2) implies

(3.3) $$||y_{n,m}|| \leq \frac{1}{1-r} \max_{m<i\leq n} ||x_i|| \ .$$

Thus, if the γ_i are bounded, the matrix

$$\begin{bmatrix} 1 & y_{n,m} \\ 0 & \hat{S}_m^n \end{bmatrix}$$

is bounded. Because $C^{n-m} = 0$ for $n > m + k$ and is trivially bounded, it then follows that $B_{n,m}$ is bounded if the β_i are bounded. Thus, it remains to consider conditions under which $||\hat{S}_n|| \leq r < 1$. Note that $\hat{S}_n$ is the companion matrix of the polynomial $\rho(\xi)/(\xi-1)$, all of whose zeros are inside the unit circle. Consider the coefficients for eq. (2.1) with constant steps. If the largest zero of $\rho(\xi)/(\xi-1)$ is $\tilde{r}$, there exists a

norm $||\cdot||_H$ such that

$$||\hat{S}||_H \leq \tilde{r} + \varepsilon = \hat{r}$$

for any $\varepsilon > 0$ where $\hat{S}$ is $\hat{S}_n$ for constant stepsizes. (Let H be a similarity transformation $\hat{S}$ to Jordan form with its nonzero off-diagonal elements equal to ε. Let $||x||_H$ be the max norm of $||Hx||$ and $||\hat{S}||_H$ the matrix norm consistent with this norm.) Now fix H and consider $||\hat{S}_n||_H$. If the coefficients α_i of a variable-step method are continuous functions of the stepsize ratios (as happens with most methods), then $||\hat{S}_n||_H$ is a continuous function of the step ratios. When all the ratios are unity, $||\hat{S}_n||_H \leq \hat{r} < 1$. Hence, for an r such that $\hat{r} < r < 1$, there exists a pair of numbers $b < 1 < B$ such that if the step ratios lie between b and B $||\hat{S}_n|| \leq r < 1$.

4. Computing b and B

This can be done once and for all for any given method, it does not have to be computed during an integration. First, the similarity transform H of $\hat{S}$ to Jordan form must be computed. (If the zeros of $\rho(\xi)$ are distinct, the Jordan form is diagonal.) Next, the function $||\hat{S}_n||_H$, which depends on the step ratios, must be formed. For any pair of values b and B, the maximum of $||\hat{S}_n||_H$ in the hypercube of step ratios between b and B can be computed (approximately). The value of b and B can be decreased and increased respectively until this maximum is any selected r such that $1 > r > \tilde{r}$. (If r is chosen closer to 1, the range between b and B will be larger, but the error constants will be greater because of the $1/(1 - r)$ factor in eq. (3.3).) For many methods one will find that b can be made very close to zero without problem as rapid step reductions in variable step methods yield methods that are

essentially one-step methods of order one or two for which the γ_i are zero. This is fortunate because it is desirable to be able to reduce the step suddenly when the solution exhibits a sharp change.

Variable Order Methods

In [2] it was shown that changing formulas "occassionally" did not affect stability. Precisely, it was shown that, for any set of strongly stable formulas $\{F_i\}$ there exists integers N_{ji} such that if at least N_{ji} steps of formula F_i are taken after a switch from formula F_j, then the combined method is stable. This result carries over to the current situation with a much simpler proof. Suppose $\hat{S}^i$ is the matrix $\hat{S}$ corresponding to formula F_i at constant stepsize. Let H_i be such that $||\hat{S}^i||_{H_i} \leq \tilde{r}_i < 1$. Choose the r_i, b_i and B_i such that $||\hat{S}^i_n||_{H_i} \leq r_i < 1$ for all step ratios in the range $[b_i, B_i]$. Now choose r such that $\max_i r_i < r < 1$. (We only consider finite sets of formula in practice. The mathematically minded must add requirements such as uniformly strongly stable to guarantee that $\sup_i r_i < 1$.) Now consider the max norm $||\cdot||$ of $\hat{S}^n_m$ where all steps are taken with method i.

$$||\hat{S}^n_m|| \leq ||H_i^{-1}|| \; ||\hat{S}^n_m||_{H_i} \; ||H_i||$$

$$\leq ||H_i^{-1}|| \; ||H_i|| \; r_i^{n-m}$$

$$\leq [||H_i^{-1}|| \; ||H_i|| \; (\frac{r_i}{r})^{n-m}] \; r^{n-m}$$

Since we have chosen $r_i < r$, there exists an integer N_i such that

$$||H_i^{-1}|| \; ||H_i|| \; (\frac{r_i}{r})^p \leq 1 \qquad \text{for all } p \geq N_i$$

Thus, if at least N_i steps are taken with formula F_i, we can bound $||\hat{S}^n_m||$ for a sequence of variable-step, variable-order formulas by Kr^{n-m} where $K = \max(||H_i^{-1}|| \; ||H_i||)$. This can easily seem to be sufficient to show that $||\hat{S}^n_m||$ is bounded as before. (The proof above yields $N_{ji} = N_i$ for all j. In practice, a smaller value of N_{ji} can be obtained by setting

$$N_{ji} = \left\lceil \frac{\log ||H_j \, H_i^{-1}||}{\log r - \log r_i} \right\rceil$$

and

$$K = \max_{i,j}(||H_j^{-1}|| \; ||H_i||).$$

Only the presentation of the proof is complicated, not the principle.)

Consequently, a practical step and order control restriction which is guaranteed to be stable for strongly stable methods is as follows:

1. If the order was changed within too few steps, stay at the current order; otherwise, consider changing the order in the next step.
2. Compute the "optimal" step and order for the next step using your favorite algorithm.
3. If the step increase is greater than permitted, use the maximum allowed.
4. If the step decrease is larger than allowed, change to a one-step method to "restart"; otherwise, take the recommended step.

(The question of restarting is the subject of a paper in preparation by this writer. It is possible to restart efficiently at high order using a one-step method which is automatically stable.)

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BIBLIOGRAPHIC DATA SHEET	1. Report No. UIUCDCS-R-78-931	2.	3. Recipient's Accession No.
4. Title and Subtitle STABILITY OF VARIABLE-STEP METHODS FOR ORDINARY DIFFERENTIAL EQUATIONS			5. Report Date July 18, 1978
			6.
7. Author(s) C. William Gear			8. Performing Organization Rept. No. UIUCDCS-R-78-931
9. Performing Organization Name and Address Department of Computer Science, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801			10. Project/Task/Work Unit No. C00-2383-0048
			11. Contract/Grant No. ENERGY/EY-76-S-02-2383
12. Sponsoring Organization Name and Address Department of Energy, 9800 South Cass Avenue, Argonne, Illinois 60439			13. Type of Report & Period Covered Research
			14.

15. Supplementary Notes

16. Abstracts

It is proved that, for any multistep formula which is strongly stable at constant stepsize, there exist constants $b < 1 < B$ such that if the ratio of adjacent steps satisfies $b \leq h_n/h_{n-1} \leq B$, the variable-step implementation of the formula is stable. A practical step-order control restriction which guarantees stability is given.

17. Key Words and Document Analysis. 17a. Descriptors

variable-step

ordinary differential equations

stability

multistep methods

variable-order

17b. Identifiers/Open-Ended Terms

17c. COSATI Field/Group

18. Availability Statement unlimited	19. Security Class (This Report) UNCLASSIFIED	21. No. of Pages 13
	20. Security Class (This Page) UNCLASSIFIED	22. Price